Excitation spectrum of d-wave Fermi surface deformation

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Several instabilities competing with the d-wave singlet pairing were proposed for high-T_c cuprates. One of them is the d-wave Fermi surface deformation (dFSD), which is generated by forward scattering. In this paper, correlation functions of the dFSD are calculated within the random phase approximation. In the normal state, the excitation spectrum shows a low energy peak, which smoothly connects to critical fluctuations of the dFSD at lower temperature. The competition with the d-wave pairing, however, blocks the critical fluctuations. The whole spectral weight is transferred to high energy and a pronounced peak appears there in the d-wave pairing state. This peak is an overdamped collective mode of the dFSD and can grow to be a resonance mode at moderate finite wavevectors.

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High-T_c cuprates are doped Mott insulators. The parent compounds are antiferromagnetic Mott insulators, which become high-T_c superconductors with carrier doping. The superconducting state does not have an isotropic gap such as BCS superconductors, but has an anisotropic gap with the d-wave symmetry.

It has been recognized that there may be several instabilities competing with the d-wave superconductivity. Effects of the antiferromagnetism may play a crucial role still in the d-wave superconducting state, and their competition was discussed using a concept of the SO(5) symmetry.[1, 2] Another idea, a self-organized one-dimensional charge order in the CuO_2 plane — spin-charge stripes hypothesis, was proposed to discuss several experimental data[3, 4] and phenomenological theories were developed.[5] Through a microscopic analysis of the two-dimensional (2D) t-J model by $1/N$ expansions for Hubbard operators, the d-wave charge density order was proposed.[6] This phase has bond currents forming staggered flux, and was discussed in different contexts.[7, 8] A similar state, called the staggered flux phase, was proposed in the SU(2) slave-boson formalism in the t-J model.[9] In this scheme, the exact SU(2) gauge symmetry at half-filling[10] was invoked also at finite doping; the underlying theoretical concept is quite different from the d-wave charge density order. All these possible competing orders come from electron-electron correlations with large momentum transfer near $\boldsymbol{q} = (\pi, \pi)$.

Recently another competing order was proposed,[11, 12] the d-wave Fermi surface deformation (dFSD).[13] The Fermi surface (FS) expands along the k_x-direction and shrinks along the k_y-direction (or vice versa). This order has to be distinguished from the above possible competing orders. The channel of this instability is forward scattering with $\boldsymbol{q} = (0, 0)$. The dFSD was first discussed for the 2D t-J model[11] and Hubbard model.[12] It was tested in several renormalization group schemes applied to the Hubbard model.[12, 14, 15] The dFSD was investigated also in perturbation theories for the Hubbard model[16, 17], in the mean-field theory for the extended Hubbard model,[18] and in phenomenological models.[19, 20, 21] In the continuum (not lattice) model FS deformation was investigated in analogy to the nematic phase in liquid crystals.[22, 23]

In accord with a result in the Hubbard model,[15] the analysis of the t-J model[11] showed that an instability of the dFSD competed with a more dominant instability, the d-wave singlet pairing, and was usually masked and not seen. However, it was shown that the presence of a small extrinsic anisotropy was sufficient to manifest the dFSD.[11] This implies that while the spontaneous instability of the dFSD does not take place, the electron system still has an appreciable susceptibility of the dFSD and is sensitive to the external anisotropy; the FS is softened.[19] This idea was invoked for LSCO systems through the consideration of band parameter dependences[11] and magnetic excitation spectra.[24]

In this letter, we investigate dynamical properties of the dFSD. Since the instability of the dFSD is signaled by divergence of its static susceptibility at $\boldsymbol{q} = 0$, we focus on the dynamical susceptibility near $\boldsymbol{q} = 0$ and calculate it within the random phase approximation (RPA). In the normal state the excitation spectrum shows a low energy peak, which smoothly connects to critical fluctuations of the dFSD at lower temperature. The critical fluctuations are, however, blocked by the more dominant d-wave pairing instability. The low energy spectral weight is suppressed and vanishes at zero temperature. Instead the spectral weight is transfered to high energy and we find a pronounced peak there. This peak is an overdamped collective mode of the dFSD and can grow to be a resonance mode at moderate finite wavevectors.

To investigate correlations of the dFSD, we take the 2D t-J model on the square lattice,

$$H = -\sum_{i,\,j,\,\sigma} t^{(l)} \tilde{c}^{\dagger}_{i\,\sigma} \tilde{c}_{j\,\sigma} + J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \qquad (1)$$

defined in the Fock space with no doubly occupied sites. Here $\tilde{c}_{i\,\sigma}$ ($\boldsymbol{S}_i$) is an electron (a spin) operator. The $t^{(l)}$ is the lth ($l \leq 2$) neighbor hopping integral, and we de-

note $t^{(1)} = t$, $t^{(2)} = t'$. The $J(>0)$ is the superexchange coupling between nearest-neighbor sites. We introduce U(1) slave-particles as $\tilde{c}^\dagger_{i\,\sigma} = f^\dagger_{i\,\sigma} b_i$, where $f_{i\,\sigma}$ (b_i) is a fermion (boson) operator that carries spin σ (charge e), and $\boldsymbol{S}_i = \frac{1}{2} f^\dagger_{i\,\alpha} \boldsymbol{\sigma}_{\alpha\,\beta} f_{i\,\beta}$ with Pauli matrix $\boldsymbol{\sigma}$. This is an exact transformation. We then decouple the interactions with the so-called resonating-valence-bond mean fields: $\chi_\tau \equiv \langle \sum_\sigma f^\dagger_{i\,\sigma} f_{i+\tau\,\sigma} \rangle$, $\langle b^\dagger_i b_{i+\tau} \rangle$, and $\Delta_\tau \equiv \langle f_{i\,\uparrow} f_{i+\tau\,\downarrow} - f_{i\,\downarrow} f_{i+\tau\,\uparrow} \rangle$, where $\boldsymbol{\tau} = \boldsymbol{r}_j - \boldsymbol{r}_i$ denotes the direction. These mean fields are assumed to be real constants independent of sites i. We approximate the boson to condense at the bottom of its band, which is reasonable at low temperature T, and obtain the following Hamiltonian:

$$H_0 = \sum_{\boldsymbol{k}} \begin{pmatrix} f^\dagger_{\boldsymbol{k}\uparrow} & f_{-\boldsymbol{k}\downarrow} \end{pmatrix} \begin{pmatrix} \xi_{\boldsymbol{k}} & -\Delta_{\boldsymbol{k}} \\ -\Delta_{\boldsymbol{k}} & -\xi_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} f_{\boldsymbol{k}\uparrow} \\ f^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix}, \quad (2)$$

with a global constraint $\sum_\sigma \langle f^\dagger_{i\sigma} f_{i\sigma} \rangle = 1 - \delta$. Here $\xi_{\boldsymbol{k}} = -2\left(F_x \cos k_x + F_y \cos k_y + 2t'\delta \cos k_x \cos k_y\right) - \mu$, $\Delta_{\boldsymbol{k}} = -\frac{3}{4} J \left(\Delta_x \cos k_x + \Delta_y \cos k_y\right)$, and $F_{x(y)} = t\delta + \frac{3}{8} J \chi_{x(y)}$, with δ being hole density and μ the chemical potential. The mean fields are determined self-consistently by minimizing the free energy. The isotropic state $\chi_x = \chi_y$ is stabilized and the d-wave singlet pairing, $\Delta_x = -\Delta_y = \Delta_0$, sets in at low T.

The advantages of this formalism[25] are (i) the phase diagram on T versus δ catches essential physics of high-T_c cuprates, (ii) magnetic excitation in actual systems was consistently described on the basis of fermiology including material dependence,[24, 26, 27] and (iii) the dFSD channel was shown to exist in the J-term,[11] which enable us study its competition with the d-wave pairing on an equal footing.

To analyze correlations of the dFSD, we define d-wave weighted fermion density,

$$\hat{\chi}_d(\boldsymbol{q}) = \sum_{\boldsymbol{k}\,\sigma} d_{\boldsymbol{k}} f^\dagger_{\boldsymbol{k}-\frac{\boldsymbol{q}}{2}\,\sigma} f_{\boldsymbol{k}+\frac{\boldsymbol{q}}{2}\,\sigma}, \quad (3)$$

with $d_{\boldsymbol{k}} = \frac{1}{2}(\cos k_x - \cos k_y)$. The spontaneous dFSD is described by $\langle \hat{\chi}_d(\boldsymbol{0}) \rangle \neq 0$, which is, however, prohibited by competition with the d-wave singlet pairing. In the d-wave singlet state, fluctuations of $\hat{\chi}_d(\boldsymbol{q})$ induce fluctuations of extended s-wave pairing.[11] To include this effect we also define

$$\hat{\Delta}_s(\boldsymbol{q}) = \sum_{\boldsymbol{k}} s_{\boldsymbol{k}} \left(f_{\boldsymbol{k}+\frac{\boldsymbol{q}}{2}\uparrow} f_{-\boldsymbol{k}+\frac{\boldsymbol{q}}{2}\downarrow} - f^\dagger_{\boldsymbol{k}-\frac{\boldsymbol{q}}{2}\uparrow} f^\dagger_{-\boldsymbol{k}-\frac{\boldsymbol{q}}{2}\downarrow} \right), \quad (4)$$

with $s_{\boldsymbol{k}} = \frac{1}{2}(\cos k_x + \cos k_y)$. Thus the correlation function forms a 2×2 matrix,

$$\boldsymbol{\kappa}_0(\boldsymbol{q},\,\omega) = \begin{pmatrix} \kappa_0^{11}(\boldsymbol{q}\,,\omega) & \kappa_0^{12}(\boldsymbol{q}\,,\omega) \\ \kappa_0^{21}(\boldsymbol{q}\,,\omega) & \kappa_0^{22}(\boldsymbol{q}\,,\omega) \end{pmatrix}, \quad (5)$$

where $\kappa_0^{12}(\boldsymbol{q}\,,\omega) = \kappa_0^{21}(\boldsymbol{q}\,,\omega)$, and

$$\kappa_0^{11}(\boldsymbol{q},\,\omega) = \frac{\mathrm{i}}{N} \int_0^\infty \mathrm{d}t \mathrm{e}^{\mathrm{i}(\omega+\mathrm{i}\Gamma)t} \langle [\hat{\chi}_d(\boldsymbol{q},\,t), \hat{\chi}_d(-\boldsymbol{q})] \rangle_0\,, \quad (6)$$

$$\kappa_0^{12}(\boldsymbol{q},\,\omega) = \frac{\mathrm{i}}{N} \int_0^\infty \mathrm{d}t \mathrm{e}^{\mathrm{i}(\omega+\mathrm{i}\Gamma)t} \langle [\hat{\chi}_d(\boldsymbol{q},\,t), \hat{\Delta}_s(-\boldsymbol{q})] \rangle_0\,, \quad (7)$$

$$\kappa_0^{22}(\boldsymbol{q},\,\omega) = \frac{\mathrm{i}}{N} \int_0^\infty \mathrm{d}t \mathrm{e}^{\mathrm{i}(\omega+\mathrm{i}\Gamma)t} \langle [\hat{\Delta}_s(\boldsymbol{q},\,t), \hat{\Delta}_s(-\boldsymbol{q})] \rangle_0\,. \quad (8)$$

Here $\hat{\chi}_d(\boldsymbol{q},\,t) = \mathrm{e}^{\mathrm{i}H_0 t} \hat{\chi}_d(\boldsymbol{q}) \mathrm{e}^{-\mathrm{i}H_0 t}$, and $\hat{\Delta}_s(\boldsymbol{q},\,t) = \mathrm{e}^{\mathrm{i}H_0 t} \hat{\Delta}_s(\boldsymbol{q}) \mathrm{e}^{-\mathrm{i}H_0 t}$. The bracket $\langle \cdots \rangle_0$ denotes an expectation value under the Hamiltonian (2), and $[\cdot\,,\,\cdot]$ is the commutator; N is the total number of lattice sites. We consider interactions in the RPA,

$$\begin{pmatrix} \kappa^{11} & \kappa^{12} \\ \kappa^{21} & \kappa^{22} \end{pmatrix}^{-1} = \begin{pmatrix} \kappa_0^{11} & \kappa_0^{12} \\ \kappa_0^{21} & \kappa_0^{22} \end{pmatrix}^{-1} - \begin{pmatrix} 3J/2 & 0 \\ 0 & 3J/2 \end{pmatrix}. \quad (9)$$

In this letter, we focus on $\kappa^{11}(\boldsymbol{q},\,\omega)$ with $\boldsymbol{q} \approx 0$, and investigate its spectral weight in both the normal state and the d-wave singlet pairing state. Full results including other components of $\boldsymbol{\kappa}$ will be shown elsewhere.[28] We take band parameters, $t/J = 4$ and $t'/t = -1/6$, for which the dFSD is known to be prominent;[11] a doping rate is fixed to $\delta = 0.10$. In Eqs.(6)-(8), the value of Γ is a positive infinitesimal and we take $\Gamma = 10^{-4}J$ (Fig. 1) or $\Gamma = 0.01J$ (Fig. 2) in numerical calculations.

Figure 1(a) shows $\mathrm{Im}\kappa^{11}(\boldsymbol{q},\,\omega)$ as a function of ω for several choices of T in the normal state at $\boldsymbol{q} = (0.01 \times 2\pi,\, 0)$. The spectral weight concentrates at low energy for all T. This is due to a property of $\mathrm{Im}\kappa_0^{11}(\boldsymbol{q},\,\omega)$ that particle-hole excitations obey the relation, $\omega = \xi_{\boldsymbol{k}+\boldsymbol{q}/2} - \xi_{\boldsymbol{k}-\boldsymbol{q}/2}$; ω becomes small for small $\boldsymbol{q}$. The low energy spectral weight increases with decreasing T and the peak position shifts closer to zero energy. This enhancement comes from the interactions in the RPA, Eq. (9), and smoothly connects to critical fluctuations of the dFSD at lower T. While the present lowest temperature ($T = 0.13J$) is much higher than the critical temperature of the dFSD ($T_{d\mathrm{FSD}} = 0.038J$), the low energy weight of $\mathrm{Im}\kappa^{11}(\boldsymbol{q},\,\omega)$ substantially increases in comparison with $\mathrm{Im}\kappa_0^{11}(\boldsymbol{q},\omega)$ as shown in the inset of Fig. 1(a). In this sense, the enhancement of the low energy peak is a precursor of collective fluctuations of the dFSD. In Fig. 1(b), we plot $\mathrm{Im}\kappa^{11}(\boldsymbol{q},\,\omega)$ for several choices of $\boldsymbol{q}$ ($\parallel$ [10]) at given T. The spectral weight spreads to higher energy with increasing $|\boldsymbol{q}|$, but the peak position stays at relatively low energy, which is due to the enhancement by the RPA. In Fig. 1(c), we summarize the excitation spectrum on the plane of ω vs. q. The shaded region is a gapless particle-hole continuum and the upper edge increases linearly with q. The peak energy of $\mathrm{Im}\kappa^{11}(\boldsymbol{q},\,\omega)$ disperses linearly with q at low q within numerical accuracy. The gradient of the q-linear becomes small at low T, which is due to the enhancement of low energy fluctuations of the dFSD. These qualitative features have been checked also along $\boldsymbol{q} \parallel$ [11].

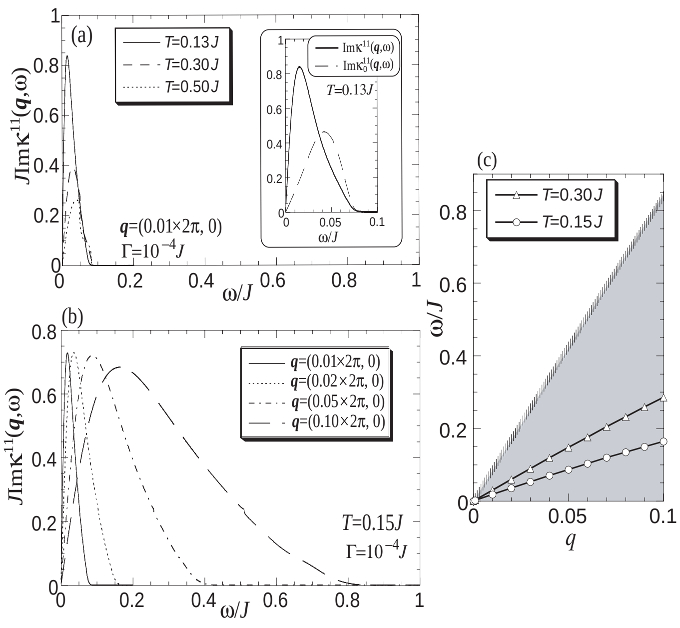

FIG. 1: Normal state. (a) ω dependence of $\mathrm{Im}\kappa^{11}(\boldsymbol{q},\,\omega)$ for several choices of T at $\boldsymbol{q} = (0.01 \times 2\pi,\, 0)$. The result at $T = 0.13J$ is compared with $\mathrm{Im}\kappa_0^{11}(\boldsymbol{q},\,\omega)$ in the inset. (b) ω dependence of $\mathrm{Im}\kappa^{11}(\boldsymbol{q},\,\omega)$ for several choices of $\boldsymbol{q}$ along the [10] direction. (c) Excitation spectrum on the plane of ω vs. q. The shaded region is a particle-hole continuum. The open circle (triangle) corresponds to the peak energy of $\mathrm{Im}\kappa^{11}(\boldsymbol{q},\,\omega)$ at a given q at $T = 0.15J$ $(0.30J)$; q is defined as $\boldsymbol{q} = (q \times 2\pi,\, 0)$.

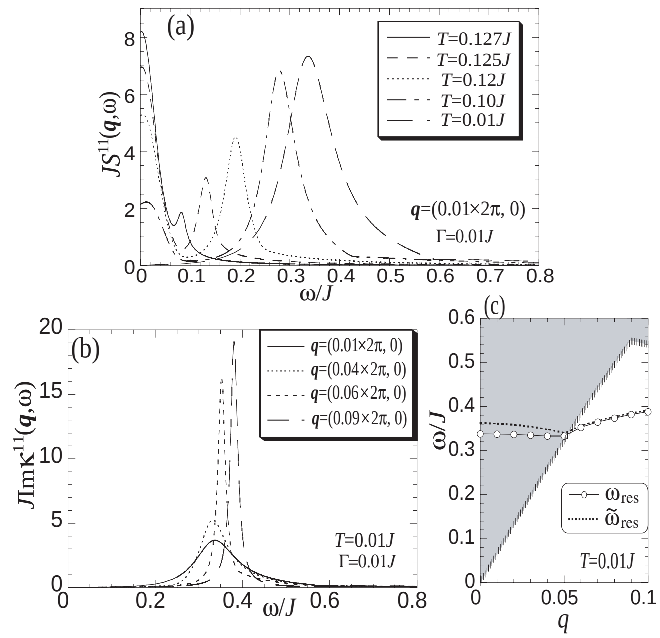

FIG. 2: d-wave pairing state. (a) ω dependence of $S^{11}(\boldsymbol{q},\,\omega)$ for several values of T at $\boldsymbol{q} = (0.01 \times 2\pi,\, 0)$. (b) ω dependence of $\mathrm{Im}\kappa^{11}(\boldsymbol{q},\,\omega)$ for several choices of $\boldsymbol{q}$ along the [10] direction ($T = 0.01J$). (c) Excitation spectrum on the plane of ω vs. q. The shaded region is a continuum of excitations. The open circle corresponds to the peak energy of $\mathrm{Im}\kappa^{11}(\boldsymbol{q},\,\omega)$, $\omega_{\rm res}$, at a given q ($T = 0.01J$); q is defined as $\boldsymbol{q} = (q \times 2\pi,\, 0)$. $\tilde{\omega}_{\rm res}$ is estimation by Eq. (10).

Further decreasing T below values shown in Fig. 1(a), the d-wave singlet pairing instability takes place, which competes with the dFSD and prohibits the spontaneous dFSD. This competition is shown in Fig. 2(a); we take the spectral function, $S^{11}(\boldsymbol{q},\,\omega) = 2\mathrm{Im}\kappa^{11}(\boldsymbol{q},\,\omega)/(1-\mathrm{e}^{-\omega/T})$, to see low energy structures also on the same scale, and plot its ω dependence for several choices of T. The low energy weight is suppressed with decreasing T and is transferred to higher energy to form a second peak there (see the results for $T \gtrsim 0.12J$). While the low energy weight vanishes at $T = 0$, the second peak grows to be a pronounced peak at low T. To see its dispersive features, we calculate the ω dependence of $\mathrm{Im}\kappa^{11}(\boldsymbol{q},\,\omega)$ for several choices of $\boldsymbol{q}$ at low T. Figure 2(b) shows that the peak width becomes narrower with $|\boldsymbol{q}|$ and a sharp peak appears at moderate $|\boldsymbol{q}|$ ($\gtrsim 0.05 \times 2\pi$). This is a resonance peak and an in-gap collective mode of the dFSD, namely a bound state (the finite peak width of the resonance is due to $\Gamma > 0$ in the numerical calculations). To see this, we calculate the gap energy of $\mathrm{Im}\kappa_0^{11}(\boldsymbol{q},\,\omega)$, namely a lower edge of a continuum of excitations, and plot it as a function of q as well as the peak energy of $\mathrm{Im}\kappa^{11}(\boldsymbol{q},\,\omega)$, $\omega_{\rm res}$, in Fig. 2(c). The lower edge increases with q and $\omega_{\rm res}$ is located inside the gap (in $q \gtrsim 0.05$), which gives rise to the resonance peak. This resonance does not appear along $\boldsymbol{q} \parallel [11]$ at least up to $\boldsymbol{q} = (0.10\times 2\pi,\, 0.10\times 2\pi)$ because of the extention of the continuum spectrum down to lower energy.

To understand the dispersion relation of the resonance, we first approximate $\kappa^{11}(\boldsymbol{q},\,\omega)$ given by Eq. (9) to $\kappa^{11}(\boldsymbol{q},\,\omega) = \kappa_0^{11}(\boldsymbol{q},\,\omega)/(1 - 3J\kappa_0^{11}(\boldsymbol{q},\,\omega)/2)$; we have checked numerically that quantitative changes by this approximation are not noticeable. The dispersion is then determined by the condition,

$$1 - \frac{3}{2}J\mathrm{Re}\kappa_0^{11}(\boldsymbol{q},\,\tilde{\omega}_{\rm res}) = 0\,. \qquad (10)$$

This equation can have two solutions for a given $\boldsymbol{q}$ and the $\tilde{\omega}_{\rm res}$ is the smaller one. We solve Eq. (10) numerically and compare $\tilde{\omega}_{\rm res}$ with $\omega_{\rm res}$ in Fig. 2(c). We see a good agreement in a moderate q-region, where the resonance appears. A poor agreement in a small q-region is due to finite weight of $\mathrm{Im}\kappa_0^{11}(\boldsymbol{q},\,\omega)$, which invalidates using Eq. (10). We, however, see that the dispersive features are well characterized by Eq. (10) in a whole q-region in Fig. 2(c).

It should be noted that Eq. (10) has solutions for any $\boldsymbol{q}$ shown in Fig. 2(c). This is due to the enhancement of $\mathrm{Re}\kappa_0^{11}(\boldsymbol{q},\,\omega)$ by the d-wave form factor in Eq. (3). Since Eq. (10) describes an in-gap collective mode at moderate $\boldsymbol{q}$, the peak of $\mathrm{Im}\kappa^{11}(\boldsymbol{q},\,\omega)$ in the small q-region is regarded as an overdamped collective mode of the dFSD.

We have investigated the RPA excitation spectrum of

the dFSD within the slave-boson mean-field approximation to the 2D t-J model. In a normal state, excitation spectrum shows a low energy peak, which connects to critical fluctuations of the dFSD at lower T. The competition with the d-wave pairing, however, blocks the critical fluctuations. The whole spectral weight is transferred to high energy and a pronounced peak appears there in the d-wave pairing state. This peak is an overdamped collective mode of the dFSD and can grow to be a resonance mode at moderate q.

While these results are obtained in the RPA, we expect that higher order corrections will not modify appreciably at least the results near $T = 0$ (Fig. 2), since the boson condenses at the bottom of its band and the U(1) gauge field describing fluctuations around the mean fields is not relevant. On the other hand, the results of Fig. 1 are obtained at finite T and a q-linear behavior of the low energy peak might not be a robust property.

Correlations of the dFSD are ingredients of both the 2D t-J model[11] and Hubbard model[12, 14, 16, 17]. Their implications for high-T_c cuprates are interesting. Since appreciable correlations of the dFSD make the electron system sensitive to an extrinsic anisotropy between the x-direction and the y-direction, even a small anisotropy can be sufficient to lead to the dFSD, possibly a quasi-1D FS in each CuO_2 plane. This possibility was proposed for Nd-doped LSCO systems.[11] Fluctuations of the dFSD in such a quasi-1D state will be investigated elsewhere.[28] In the absence of a (static) xy-spatial anisotropy, the present theory is applicable and we expect the excitation spectrum Fig. 1(c) in the normal state and Fig. 2(c) in the d-wave pairing state.[29] As a direct test, however, conventional optical methods are not sufficient, since they measure a quantity with $\boldsymbol{q} = 0$ and will not reach a finite $\boldsymbol{q}$-region, especially the region where the resonance mode is predicted. Indirectly, searching some phonon anomalies may be promising since fluctuations of the dFSD are expected to couple with a lattice degree of freedom. However, we do not have calculations on such coupled systems at present.

Fluctuations of the dFSD should not be confused with those of spin-charge stripes.[3, 4] (i) The dFSD is generated by forward scattering while formation of spin-charge stripes requires an interaction with large momentum transfer. The underlying physics is different. (ii) Fluctuations of the dFSD are relevant in systems near the breaking of the square lattice symmetry while stripe fluctuations make sense in systems near translational symmetry breaking.

While some hidden orders are often discussed in the connection with the pseudogap,[30] correlations of the dFSD are not related directly to the pseudogap in the slave-boson scheme.[25] However, their effects may contribute to pseudogap behaviors additively, since the present FS deformation has the d-wave symmetry, the same symmetry as the pseudogap.

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